DD2434 – Advanced Machine Learning

Lecture 2: **Probabilistic approach – fundamentals**

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Course content

- Aims and scope of this part of the course

I. Probabilistic regression

- *Lecture 2:* Probabilistic approach (objects and inference)
- *Lecture 3:* Linear regression
- *Lecture 4:* Kernels and introduction to Gaussian processes
- *Lecture 5:* Gaussian processes

II. Probabilistic representation learning

- *Lecture 6:* Representation learning

Course content

- Learning activities
  - 5 lectures
  - 2 exercise sessions (fun with Gaussians ;-))
  - 1 assignment
  - project based on a research paper

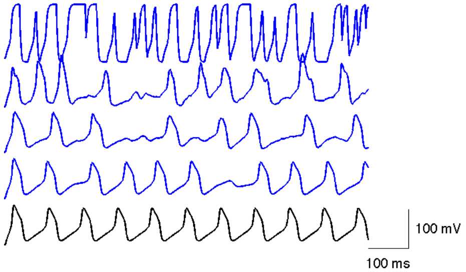
Short outline for today

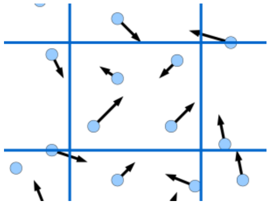
1. Introduction – why is probability theory relevant in ML?
2. Probabilistic approach to ML – principles (*recap*).
3. Probability basics (tbc).

Introduction

Probabilistic approach

- Ubiquitous nature of uncertainty
  - imprecision, noise in data,
  - errors , missing information/data
  - gaps in knowledge, simplified description





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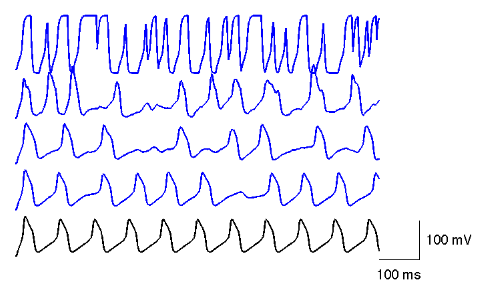

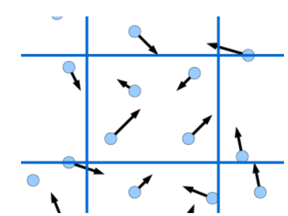

"The theory of probabilities is at bottom nothing but common sense reduced to calculus; it enables us to appreciate with exactness that which accurate minds feel with a sort of instinct for which of times they are unable to account." (Laplace)

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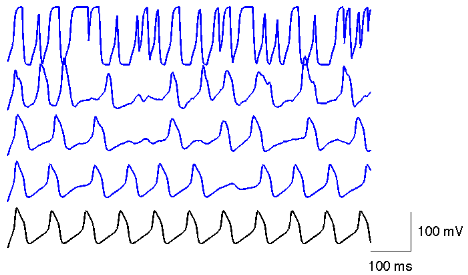
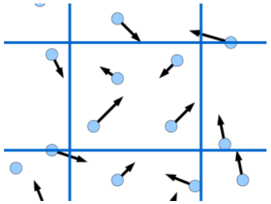


- Probability theory provides a framework for modelling, reasoning etc. under uncertainty
  - unified, universal, intuitive, interpretable
  - beyond randomness, it is about uncertainty!
  - p. distributions as carriers or information (Jaynes, 2003)



Probabilistic perspective in ML

- Statistical ML: constructing stochastic models
  - fully probabilistic description and inference
  - theoretical assumptions, mathematical tractability, rigour
  - parameters estimated from observed data (learning)
  - interpretability and extra insights
  - machinery to propagate and account for uncertainty effects

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BUT: *can be very hard for large-scale problems* and

difficult to derive solutions in a closed form

Probabilistic perspective in ML

- Statistical ML: constructing stochastic models
  - fully probabilistic description and inference
  - t … igour
  - p
  - i
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> “ *(statistical ML) provides the basis for learning algorithms that directly manipulate probabilities, as well as a framework for analyzing the operation of other algorithms that do not explicitly manipulate probabilities.*” Mitchell

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)

Probabilistic perspective in ML

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  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
    - product and sum probability rules, Bayesian theorem

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathcal{D})}$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
    - product and sum probability rules, Bayesian theorem
    - the power of marginalisation

$$p(x_1, x_2 .., x_{n-1}) = \int p(x_1, x_2, .., x_n) dx_n$$

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Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
  - Combine uncertain knowledge with data to reduce uncertainty (based on evidence from observations)
    - batch or sequence where posterior is iteratively updated

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
  - Combine uncertain knowledge with data to reduce uncertainty (based on evidence from observations)
  - Two levels of inference:

    parameter estimation and model selection (see Lecture 3)

Other ML approaches

- Probabilistic narration is not the only one in ML

concept learning
based on symbolic
representations
(inductive learning
hypothesis)

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concept learning (inductive learning hypothesis)

rule learning (e.g., Inductive Logic Programming)

and rule-based learning

instance based learning (k-means)

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rule learning (e.g., Inductive Logic Programming) and rule-based learning

computational learning theory (PAC or Mistake-Bound learning model)

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decision tree learning

reinforcement learning

Other ML approaches

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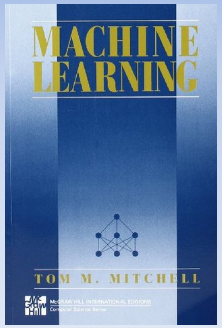
You also may have heard about

- artificial neural networks, deep architectures
- search heuristics, e.g. genetic algorithms
- support vector machines

  (origins in comp learning theory)
- etc.



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ML comes in many flavours

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Back to the probabilistic mindset

Bayesian vs frequentist perspective

I. Probability is a measure of belief (plausibility)

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VI. Probability of a hypothesis given the data (posterior distribution).

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VI. Probability of the data given hypothesis (likelihood, sampling dist.).

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Why isn't everyone Bayesian? *(Efron, 1986)*

Learning as inference – recap (*c.f.* DD2431, L6 G. Salvi)

- Learning distributions
  - *"integrating data with domain knowledge of model environment"*

$$y = f(x) : X \to Y$$

$$\{(x_1, t_1), \ldots, (x_N, t_N)\}$$

Learning implies the parameter identification of the model adopted to account for the mapping $X \to Y$

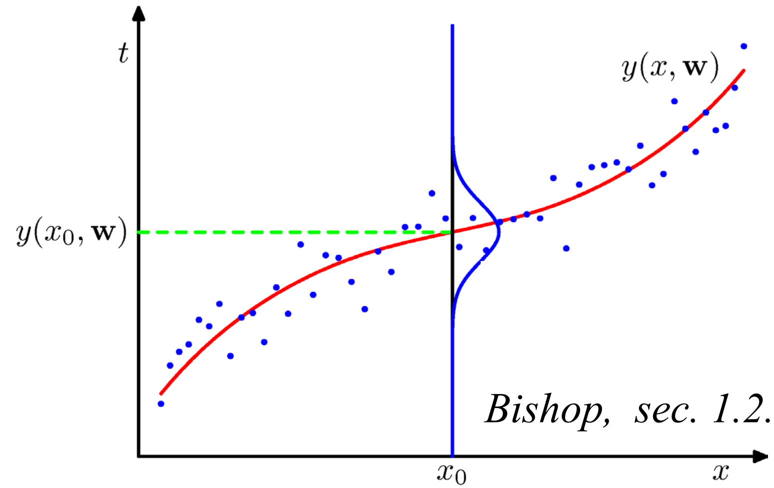
Inference is about using the model to predict the output corresponding to the sample input: *what is the model's response for* $x = x^*$?

Learning as inference – recap

- Learning distributions
  - curve-fitting example: $y(x, \mathbf{w}) : X \to Y$ (let's assume polynomial)

$$t = y(x,\mathbf{w}) + \varepsilon$$

observations $\{(x_i, t_i): i=1,..,N\}$: $\mathbf{x} = (x_1, \ldots, x_N)^{\mathrm{T}}$, $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$



Bishop, sec. 1.2.5

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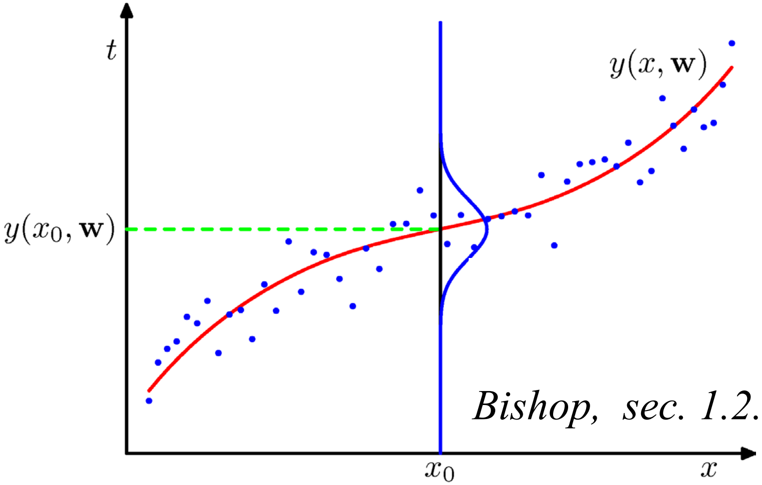
<u>Remarks about notation:</u>

1) here we deal with one-dim input, x and output, t
2) parameters $\mathbf{w}$ still constitute a vector (e.g. could be polynomial coefficients)
3) $\mathbf{x}$ and $\mathbf{t}$, refer to the collection of all inputs and outputs, conceptually corresponding to D_x and D_t, but in the vector form, so $\mathbf{x} \to \mathbf{t}$.



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  - probabilistic framework

$p(\mathbf{w})$ – a prior probability distribution

$p(\mathcal{D} \mid \mathbf{w})$ – the likelihood function for $\mathcal{D} = \mathbf{t}$
(not a probability distrib. over $\mathbf{w}$, just a conditional probability)

$p(\mathbf{w} \mid \mathcal{D})$ – a posterior probability

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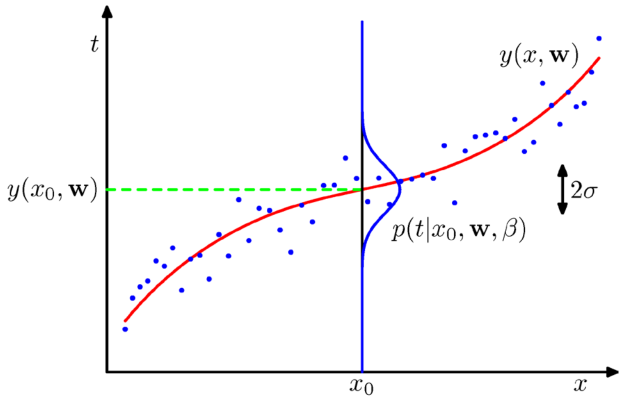

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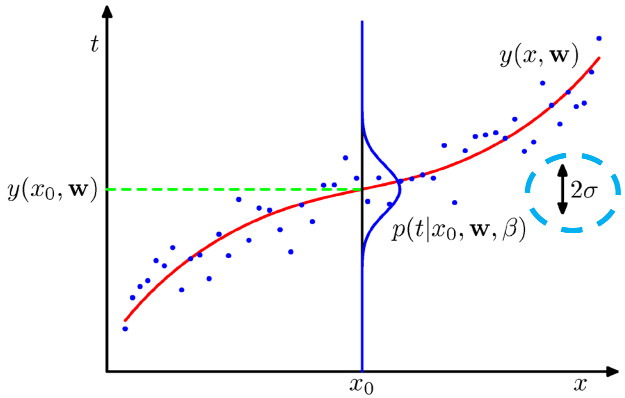
Uncertainty (noise) in target data:

$$p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x, \mathbf{w}), \beta^{-1})$$

↑

precision



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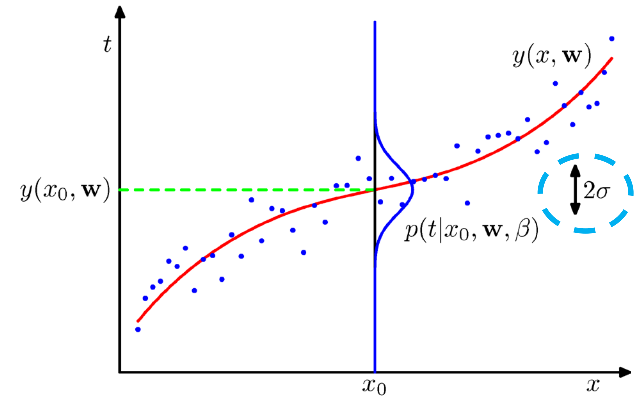
$$\underbrace{p(t \mid x, \mathbf{w}, \beta)}_{\text{predictive distribution}} = \mathcal{N}(t \mid y(x,\mathbf{w}), \beta^{-1})$$

predictive **distribution**
(not a point estimate)

precision



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SOLUTION 1

We want to find parameters to be able to use predictive distribution, $p(t|x)$, and infer the target:

$$\mathrm{E}[t \mid x] = \int t\, p(t \mid x, \mathbf{w}_{\mathrm{opt}}, \beta_{\mathrm{opt}})\,\mathrm{d}t$$

Learning as inference – recap

So, we follow the max likelihood approach

ML function for t (i.i.d.) under Gaussian noise $p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x, \mathbf{w}), \beta^{-1})$

$$p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid y_n(x_n, \mathbf{w}), \beta^{-1})$$

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The log-likelihood:

$$\boxed{\ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)}$$

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Still, input x is one-dim and $\mathbf{x}$ & $\mathbf{t}$ refer to the collection of all data points.

Learning as inference – recap

Maximum likelihood (ML) estimate:

Maximise $$\ln p(\mathbf{t}\,|\,\mathbf{x},\mathbf{w},\beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w})-t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)$$

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$$\mathbf{w}_{\mathrm{ML}} = \arg\min_{\mathbf{w}} \left\{ \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 \right\}$$

the sum-of-squares error function

under the assumption of Gaussian noise : $p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x, \mathbf{w}), \beta^{-1})$

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$$\mathbf{w}_{\mathrm{ML}} = \arg\min_{\mathbf{w}} \left\{ \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}) - t_n \}^2 \right\}$$

$$\beta_{\mathrm{ML}}^{-1} = \frac{1}{N} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}_{\mathrm{ML}}) - t_n \}^2$$

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$$\boxed{t_{out} = \mathrm{E}[t\,|\,x_{in}] = \int t\,p(t\,|\,x_{in},\mathbf{w}_{\mathrm{ML}},\beta_{\mathrm{ML}})\,\mathrm{d}t}$$

Learning as inference – recap

- Learning distributions
  - curve-fitting example: $y(x,\mathbf{w}): X \rightarrow Y$ (let's assume polynomial)

$$t = y(x,\mathbf{w}) + \varepsilon$$

Solution 2

Parameters of the model could also be random variables with a prior distribution, $p(\mathbf{w} \mid \alpha) = \mathcal{N}(\mathbf{w} \mid \mathbf{0}, \alpha^{-1}\mathbf{I})$

Now, we must **maximise the posterior** $p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)$, i.e. find the most probable $\mathbf{w}$ given data:

$$\max p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta)\ p(\mathbf{w} \mid \alpha)$$

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Again, $\mathbf{x}$ & $\mathbf{t}$ refer to the data collection, not individual input or outputs

Learning as inference – recap

Maximum posterior (MAP) estimate:

Maximise $\ln p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)$

$$\downarrow$$

$$\boxed{\mathbf{w}_{\text{MAP}} = \arg\min_{\mathbf{w}} \left\{ \frac{\beta}{2} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}) - t_n \}^2 + \frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \right\}}$$

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BUT: Solutions 1 (ML) and 2 (MAP) give point estimates of $\mathbf{w}$

Learning as inference – Bayesian view

Instead of estimating “optimal” parameters $\mathbf{w}$, let’s integrate over all values of $\mathbf{w}$ (let’s make use of the distribution)

Marginalisation:

$$\underbrace{p(t \mid x, \mathbf{x}, \mathbf{t}, \alpha, \beta)}_{\text{predictive}} = \int \underbrace{p(t \mid x, \mathbf{w}, \beta)}_{\text{“noise” model}} \underbrace{p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)}_{\text{posterior}} \, \mathrm{d}\mathbf{w}$$

We assume we know what α and β are.

Learning as inference – Bayesian view

Instead of estimating "optimal" parameters $\mathbf{w}$, let's integrate over all values of $\mathbf{w}$ for our linear model $y = \sum_{i=0}^{M} w_i \phi_i(x)$

For a one-dim polynomial model: $\phi_i(x) = x^i$ (order M-1)

Learning as inference – Bayesian view

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For a one-dim polynomial model: $\phi_i(x) = x^i$

$$p(t \mid x, \mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}\left(t \mid m(x), s^2(x)\right) \quad \begin{cases} m(x) = \beta \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) t_n \\ s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S}\, \boldsymbol{\phi}(x) \end{cases}$$

$$\mathbf{S}^{-1} = \alpha \mathbf{I} + \beta \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^{\mathrm{T}}$$

$$\boldsymbol{\phi}(x) = (\phi_0(x), \ldots, \phi_M(x))$$

Learning as inference – summary

In summary:

To use a predictive distribution and infer the output t for the given input x_{in} ....

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To use a predictive distribution and infer the output t for the given input x_{in} ……..

…..ML and MAP approaches produce point estimates of $\mathbf{w}$

$$\text{ML}: \quad \mathcal{D} \rightarrow \mathbf{w}_{\text{ML}}$$

$$\text{MAP}: \quad \mathcal{D}, p(\mathbf{w}) \rightarrow \mathbf{w}_{\text{MAP}}$$

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.....in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

$$\text{Bayes:} \quad \mathcal{D}, p(\mathbf{w}) \rightarrow p(\mathbf{w} \mid \mathcal{D})$$

c.f. DD2431, Lecture 6, G. Salvi

Learning as inference – summary

In summary:

To use a predictive distribution and infer the output t for the given input x_{in} ....

.....ML and MAP approaches produce point estimates of $\mathbf{w}$

$$\text{ML}: \quad \mathcal{D} \to \mathbf{w}_{\text{ML}}$$

$$\text{MAP}: \quad \mathcal{D}, p(\mathbf{w}) \to \mathbf{w}_{\text{MAP}}$$

Use $p(t \mid x_{in}, \mathbf{w}_{\text{ML}})$ or $p(t \mid x_{in}, \mathbf{w}_{\text{MAP}})$ for prediction.

.....in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

$$\text{Bayes}: \quad \mathcal{D}, p(\mathbf{w}) \to p(\mathbf{w} \mid \mathcal{D})$$

Marginalise over $\mathbf{w}$:

$$p(t \mid \mathcal{D}) = \int p(t \mid x_{in}, \mathbf{w})\, p(\mathbf{w} \mid \mathcal{D})\, \mathrm{d}\mathbf{w}$$

Learning as inference – summary

In summary:

To use a predictive distribution and infer the output t for the given input x_{in} ……..

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Frequentist philosophy

$p(t \mid x_{in}, \mathbf{w}_{\text{MAP}})$ for prediction.

…..in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

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Bayesian philosophy

$$p(t \mid \mathcal{D}) = \int p(t \mid x_{in}, \mathbf{w})\, p(\mathbf{w} \mid \mathcal{D})\, \mathrm{d}\mathbf{w}$$

Inference and decision (classification)

The ***inference*** stage of classification $\mathcal{D} \rightarrow p(C_k, \mathbf{x}), k = 1,..,K$

Model the inputs $\mathbf{x}$ and outputs C

$$\left.\begin{array}{l} p(\mathbf{x} \mid C_k) \\ p(C_k) \end{array}\right\} \text{ for each class } C_k \qquad p(\mathbf{x}, C_k)$$

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k)\, p(C_k)}{p(\mathbf{x})}$$

$$p(\mathbf{x}) = \sum_k p(\mathbf{x} \mid C_k)\, p(C_k)$$

Inference and decision (classification)

The ***inference*** stage of classification $\mathcal{D} \rightarrow p(C_k, \mathbf{x}), k = 1,..,K$

Remarks:
1) K classes
2) $\mathbf{x}$ – multi-dim input feature vector

Model the inputs $\mathbf{x}$ and outputs C

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GENERATIVE approach

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GENERATIVE approach

Solve first the inference problem of determining posteriors for each class without modelling $p(C_k, \mathbf{x})$ or $p(\mathbf{x} \mid C_k)$

$$p(C_k \mid \mathbf{x})$$

DISCRIMINATIVE approach

Generative vs discriminative approach

What are the virtues of the generative approach?

- The parameters are estimated separately for each class (no need to retrain the model when new classes are added)
- Rather straightforward to fit in a Bayesian framework (but it depends on the problem, sometimes discriminative function can be easier to optimise)

Generative vs discriminative approach

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- Easy and elegant way of handling missing or unlabelled data
- Generative model allows for….. generating data

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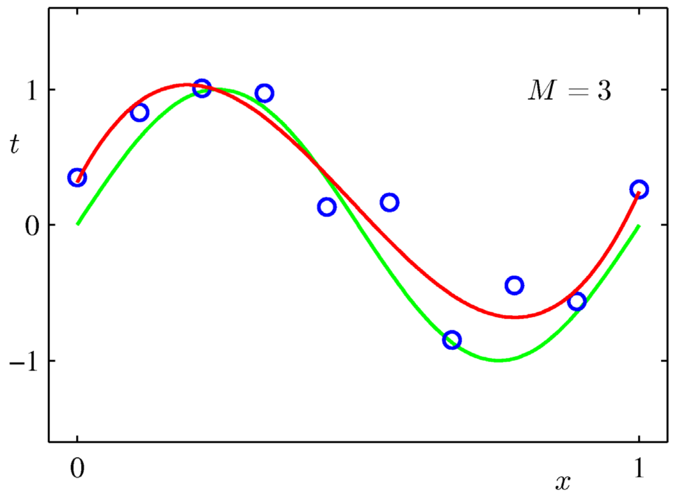
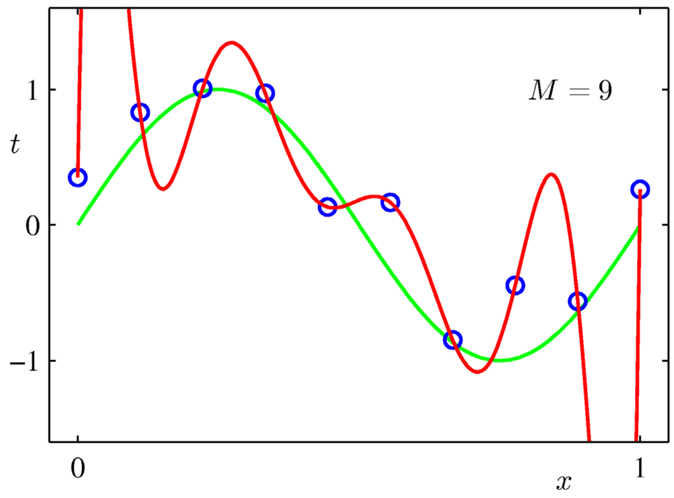
  -> generative models can be run “backwards”
- BUT: discriminative models tend to be more accurate (less vulnerable to assumptions)

Model complexity

- Overfitting



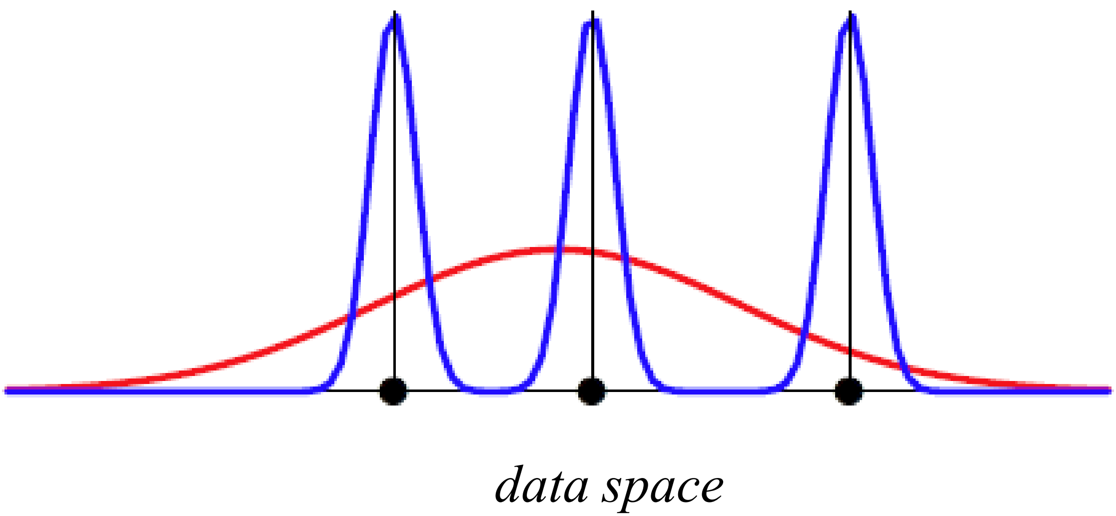


Bishop, sec. 1.1

Please recall from Lecture 1 (J. Lagergren)

Model complexity

- Overfitting



The likelihood can be arbitrarily large by adding parameters.

Please recall from Lecture 6, DD2431 (G. Salvi)

Frequentist viewpoint – bias-variance dilemma

- Maximum Likelihood estimate for linear regression corresponds to minimising loss $L(t, y(\boldsymbol{x})) = \{y(\boldsymbol{x}) - t\}^2$

Remarks about notation:

1) $\boldsymbol{x}$ can be a multi-dim input
2) $y(\boldsymbol{x})$ really is $y(\boldsymbol{x},\boldsymbol{w})$ that depends on parameters $\boldsymbol{w}$

Frequentist viewpoint – bias-variance dilemma

- Maximum Likelihood estimate for linear regression corresponds to minimising loss $L(t, y(\boldsymbol{x})) = \{y(\boldsymbol{x}) - t\}^2$

- The expected loss, L, to be minimised looks then as follows:

$$\mathbb{E}[L] = \iint \{y(\boldsymbol{x}) - t\}^2 \, p(\boldsymbol{x}, t) \, d\boldsymbol{x} \, dt$$

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$$\Downarrow$$

$$\mathbb{E}[L] = \int \{y(\boldsymbol{x}) - \mathbb{E}_t[t \mid \boldsymbol{x}]\}^2 \, p(\boldsymbol{x}) \, d\boldsymbol{x} + \int \mathrm{var}[t \mid \boldsymbol{x}] \, p(\boldsymbol{x}) \, d\boldsymbol{x}$$

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noise on the data,
independent of the regressor $y(\boldsymbol{x})$

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optimal prediction to be accounted for by our regression model $y(\boldsymbol{x})$: $h(\boldsymbol{x}) = \mathbb{E}_t[t \mid \boldsymbol{x}]$

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$$\{y(\boldsymbol{x}) - h(\boldsymbol{x})\}^2$$

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optimal prediction to be accounted for by our regression model $y(\boldsymbol{x})$: $h(\boldsymbol{x}) = \mathbb{E}_t [t \mid \boldsymbol{x}]$

h is the underlying model (data generating mechanism) that we want to approximate.

$$\mathbb{E}[L] = \int \{y(\boldsymbol{x}) - \mathbb{E}_t[t \mid \boldsymbol{x}]\}^2 p(\boldsymbol{x})\, d\boldsymbol{x} + \underbrace{\int \mathrm{var}[t \mid \boldsymbol{x}]\, p(\boldsymbol{x})\, d\boldsymbol{x}}_{\text{noise on the data, independent of the regressor } y(\boldsymbol{x})}$$

$$\{y(\boldsymbol{x}) - h(\boldsymbol{x})\}^2$$

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$$\mathbb{E}[L] = \underbrace{\int \{y(\boldsymbol{x}) - \mathbb{E}_t[t \mid \boldsymbol{x}]\}^2 p(\boldsymbol{x})\, d\boldsymbol{x}}_{\text{has to be minimised}} + \underbrace{\int \operatorname{var}[t \mid \boldsymbol{x}]\, p(\boldsymbol{x})\, d\boldsymbol{x}}_{\text{noise on the data, independent of the regressor } y(x)}$$

Frequentist approach

- Find optimal parameters for y using data D

$$\int_{\mathcal{D}} \{y(\boldsymbol{x}) - h(\boldsymbol{x})\}^2 p(\boldsymbol{x})\, d\boldsymbol{x} \quad \rightarrow \quad \min \{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\}^2$$

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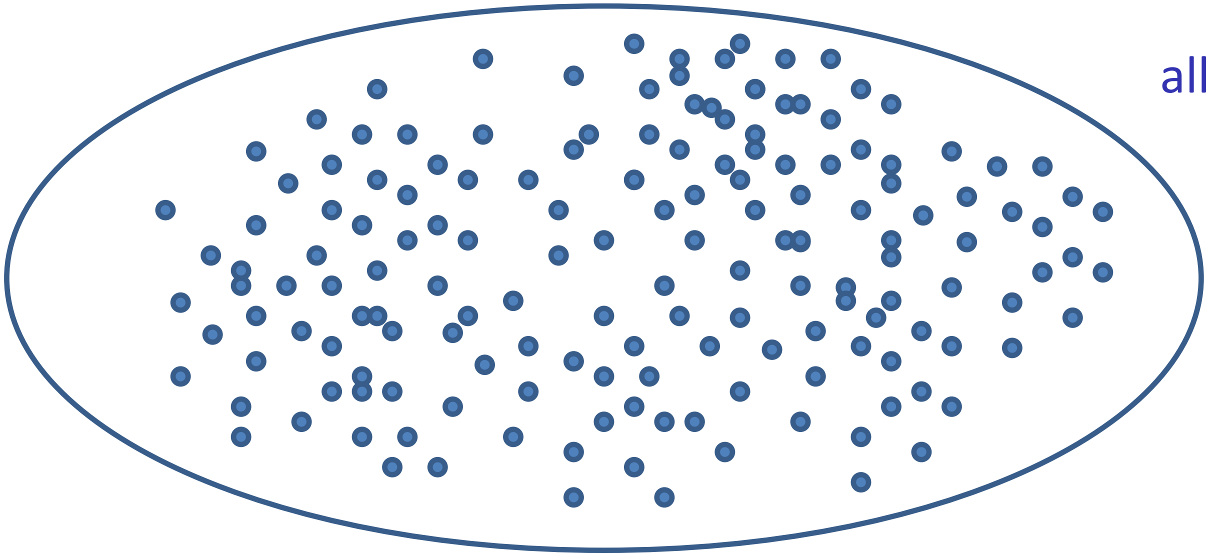
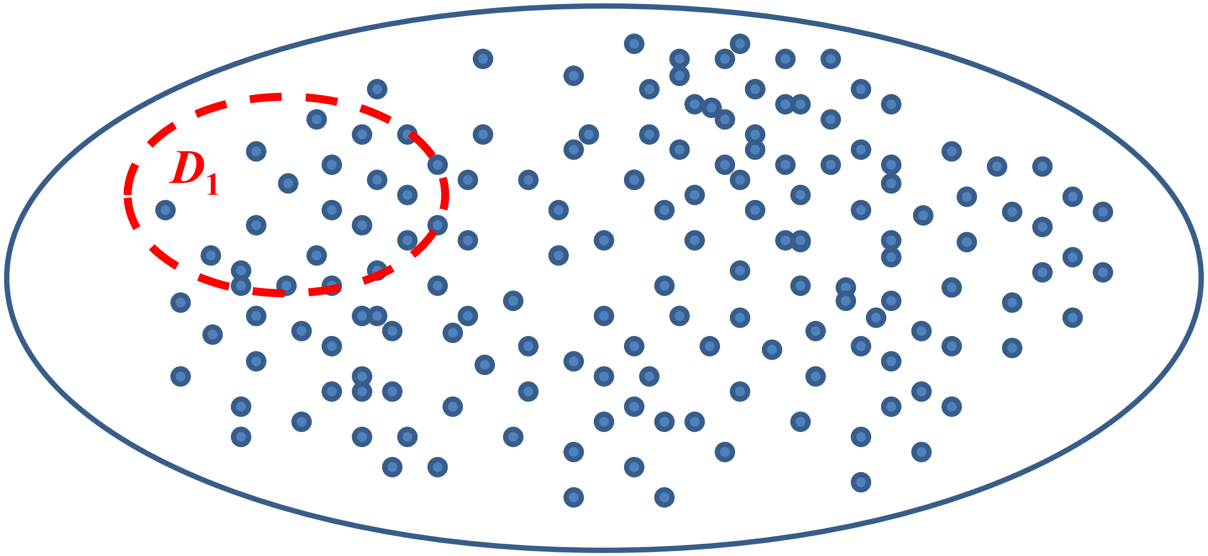


all datasets D

Frequentist approach

- Find optimal parameters for y using data D

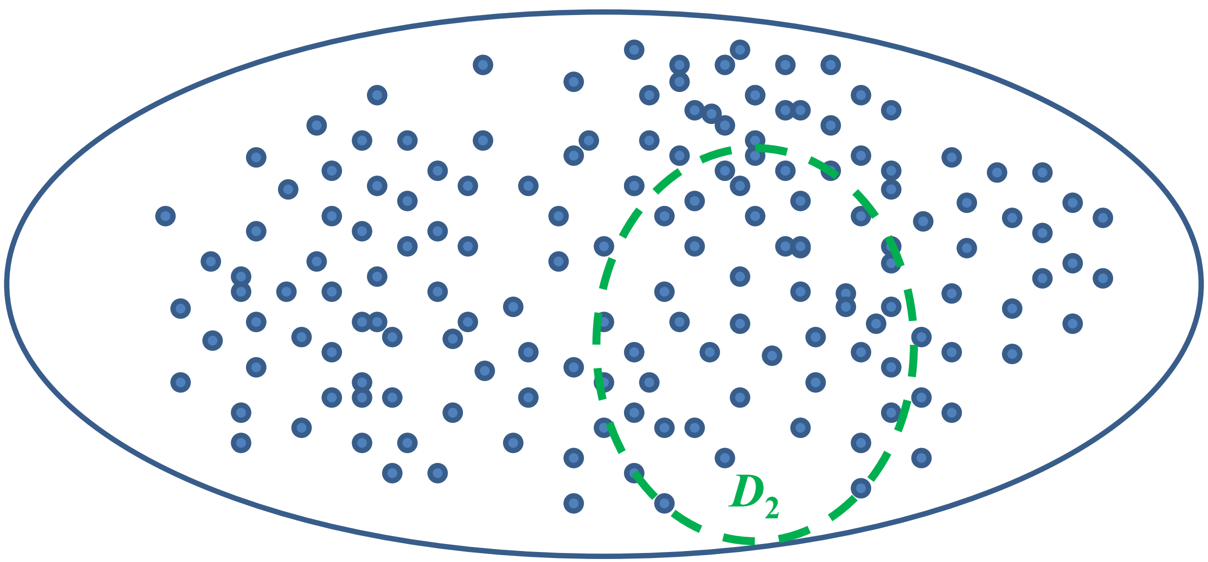
$$\min\left\{y(\boldsymbol{x};\mathcal{D}_1)-h(\boldsymbol{x})\right\}^2$$



Frequentist approach

- Find optimal parameters for y using data D

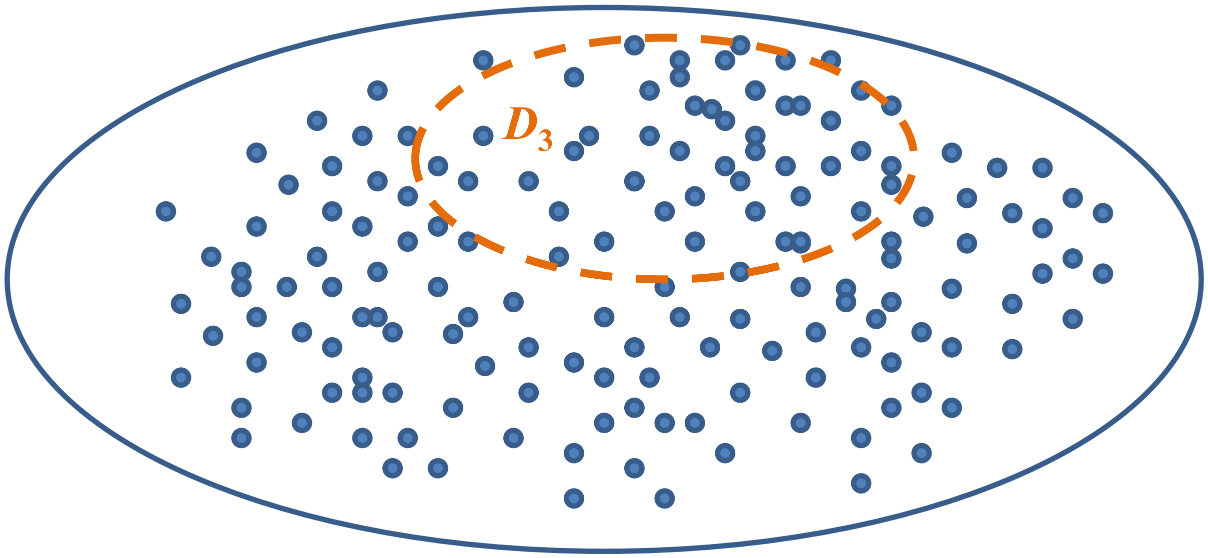
$$\min\left\{y(\boldsymbol{x};\mathcal{D}_2)-h(\boldsymbol{x})\right\}^2$$



Frequentist approach

- Find optimal parameters for y using data D

$$\min\left\{ y(\boldsymbol{x}; D_3) - h(\boldsymbol{x}) \right\}^2$$



Bias-variance decomposition

Expected value over all possible datasets D

$$\mathbb{E}[L] = \mathbb{E}_{\mathcal{D}}\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 + \int \mathrm{var}\left[t \mid \boldsymbol{x}\right] p(\boldsymbol{x})\, d\boldsymbol{x}$$

Bias-variance decomposition

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Taking frequentist perspective of fixing the model for specific data:

$$\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 = \left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] + \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2$$

Bias-variance decomposition

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…and then averaging all possible data $\mathbb{E}_{\mathcal{D}}$

$$\mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2\right] = \left\{\mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2 + \mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right]\right\}^2\right]$$

Bias-variance decomposition

Expected value over all possible datasets D

$$\mathbb{E}[L] = \mathbb{E}_{\mathcal{D}}\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 + \int \operatorname{var}\left[t \mid \boldsymbol{x}\right] p(\boldsymbol{x})\, d\boldsymbol{x}$$

$$\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 = \left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] + \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2$$

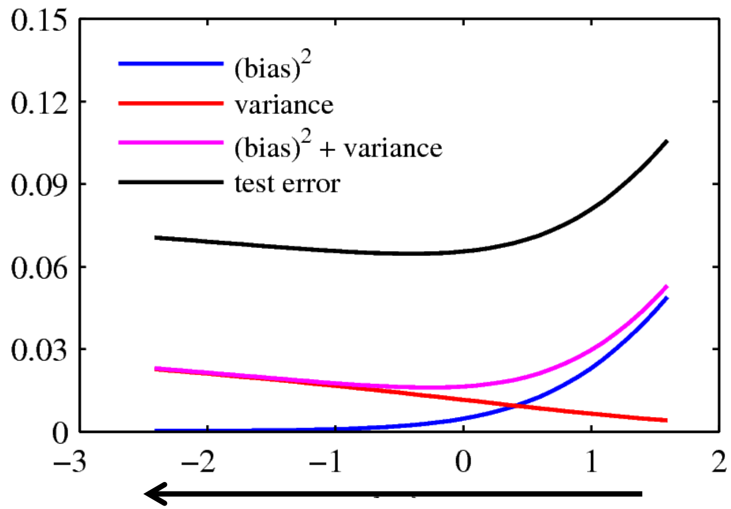
$$\mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2\right] = \underbrace{\left\{\mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right]\right\}^2\right]}_{\text{variance}}$$

Bias-variance dilemma: model complexity

Expected value over all possible datasets D

$$\mathbb{E}_{\mathcal{D}}[L] = \mathbb{E}_{\mathcal{D}}\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 + \int \operatorname{var}\left[t \mid \boldsymbol{x}\right] p(\boldsymbol{x})\, dx$$

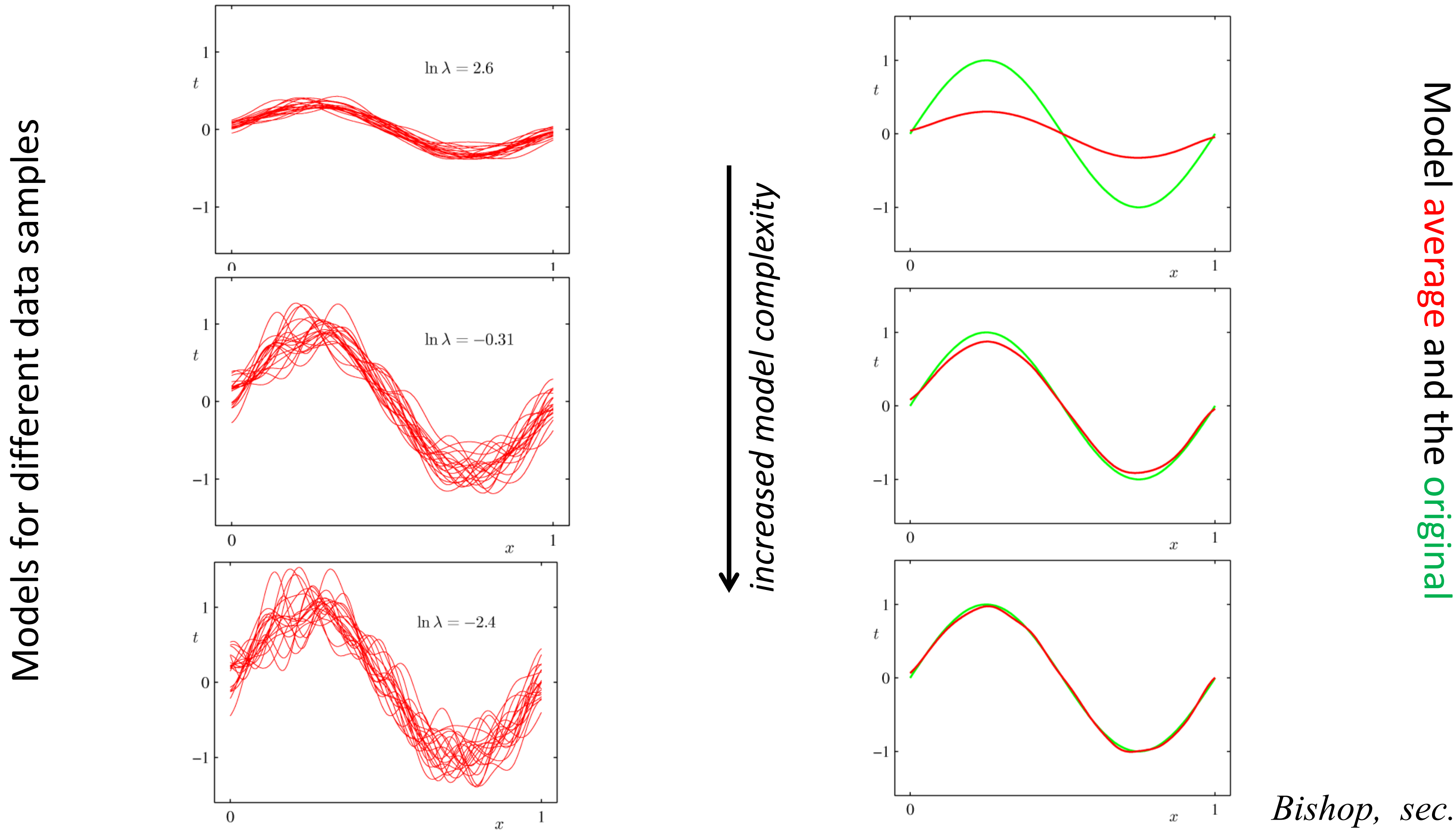
$$\mathbb{E}[L] = (\text{bias})^2 + \text{variance} + \text{noise}$$



increased model complexity

Bishop, sec. 3.2

Bias-variance: illustrative example



Bishop, sec. 3.2

Model selection (*c.f.* L1, J. Lagergren)

- Occam's razor – *"Accept the simplest explanation that fits the data."*

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Model selection (*c.f.* L1, J. Lagergren)

- Occam's razor – *"Accept the simplest explanation that fits the data."*
- Frequentist approach with maximum likelihood
  - bias-variance dilemma
  - need to control the model's complexity
    - regularisation
    - correction for the bias of ML estimates (AIC, BIC)
    - empirical estimate of generalisation error on a hold-out set (validation, resampling)
    - structural risk minimization (SRM) (minimise upper bound on the true risk), see also VC dimension (statistical learning theory)

Model selection (*c.f.* L1, J. Lagergren)

- Occam's razor – *"Accept the simplest explanation that fits the data."*
- Frequentist approach with maximum likelihood
  - bia
  - ne
    - –
    - –
    - –
    - structural risk minimization (SRM) (minimise upper bound on the true risk), see also VC dimension

Bayesian model selection

(to appear in Lecture 3)

- the second inference stage to compare models the Bayesian way
- Bayes' factor and complexity penalisation (relies on the evidence approximation)

Selected fundamental concepts

1. Introduction – why is probability theory relevant in ML?
2. Probabilistic approach to ML – principles (*recap*).
3. **Probability basics.**

Selected fundamental concepts

1. Introduction – why is probability theory relevant in ML?
2. Probabilistic approach to ML – principles (*recap*).
3. **Probability basics.**

You should really be familiar with the fundamentals!

Please take a closer look at sec. 1.2, 2.1-2.4 in (Bishop, 2006)

Here, we will VERY briefly mention

- the multivariate Gaussian distribution
- Central Limit Theorem

Selected fundamental concepts

1. Introduction – why is probability theory relevant in ML?
2. Probabilistic approach to ML – principles (*recap*).
3. **Probability basics.**

<u>You should really be familiar with the fundamentals!</u>

Plea

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More to come in
the first practical session

focus on sec.2.3- 2.4 (Bishop)

Central Limit Theorem

The Gaussian (normal) distribution

$$\mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{L/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

$\mathbf{x} \in \mathbb{R}^L$

$\boldsymbol{\mu}$ – mean vector, $\mathbb{R}^L$

$\boldsymbol{\Sigma}$ – covariance matrix , L x L

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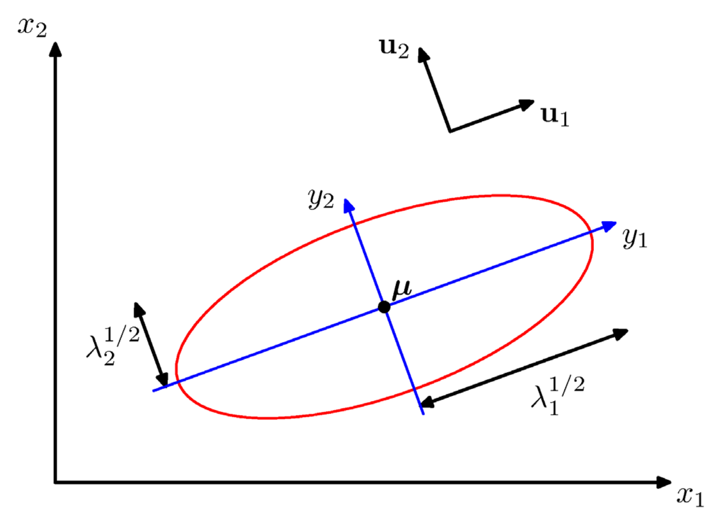
$\mathbf{x} \in \mathbb{R}^L$

$\boldsymbol{\mu}$ – mean vector, $\mathbb{R}^L$

$\boldsymbol{\Sigma}$ – covariance matrix , L x L

$$\boldsymbol{\Sigma} = \sum_{i=1}^{D} \lambda_i \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}}$$



Bishop, sec. 2.3

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$\mathbf{x} \in \mathbb{R}^L$

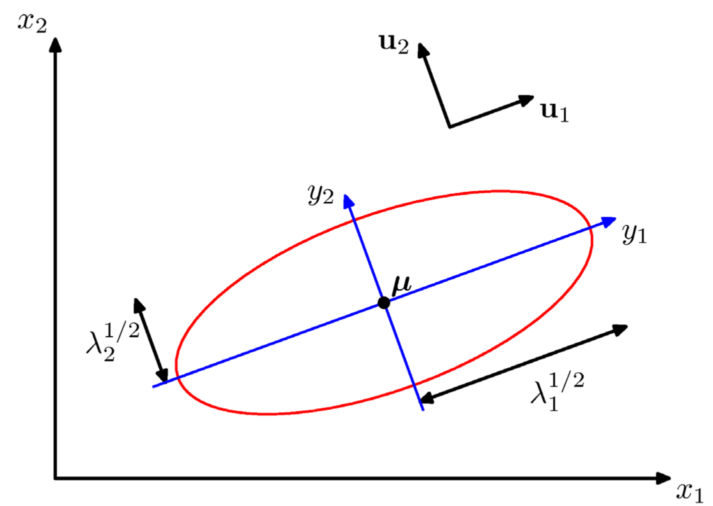
$\boldsymbol{\mu}$ – mean vector, $\mathbb{R}^L$

$\boldsymbol{\Sigma}$ – covariance matrix , L x L

$$\mathbb{E}[\mathbf{x}] = \int \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})\, \mathbf{x}\, d\mathbf{x} = \boldsymbol{\mu}$$

$$\mathbb{E}\left[\mathbf{x}\mathbf{x}^{\mathrm{T}}\right] = \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}} + \boldsymbol{\Sigma}$$

$$\mathrm{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right] = \boldsymbol{\Sigma}$$



Bishop, sec. 2.3

The Gaussian distribution

Two-dimensional (2D) case, i.e. $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

<u>Remark about notation</u>:

Unlike in the beginning, where x_i corresponded to the i-th realisation of one-dim r.v. x, **here** x_1 and x_2 correspond to one-dimensional variables that constitute two-dim r.v. $\mathbf{x}$.

The Gaussian distribution

Two-dimensional (2D) case, i.e. $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

$$\mu_i = \mathbb{E}[x_i]$$

$$\sigma_{i,j} = \sigma(x_i, x_j) = \mathbb{E}\left[\left(x_i - \mathbb{E}[x_i]\right)\left(x_j - \mathbb{E}[x_j]\right)^{\mathrm{T}}\right]$$

$$\sigma_{i,i} = \sigma_i^2 = \mathrm{var}[x_i]$$

The Gaussian distribution

Two-dimensional (2D) case, i.e. $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

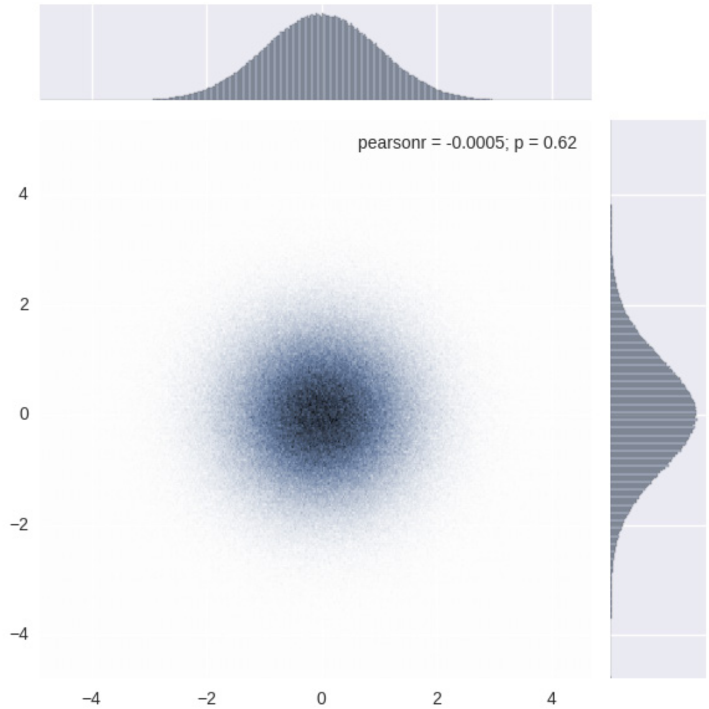
$$\mu_i = \mathbb{E}[x_i]$$

$$\sigma_{i,j} = \sigma(x_i, x_j) = \mathbb{E}\left[\left(x_i - \mathbb{E}[x_i]\right)\left(x_j - \mathbb{E}[x_j]\right)^{\mathrm{T}}\right]$$

$$\sigma_{i,i} = \sigma_i^2 = \mathrm{var}[x_i]$$

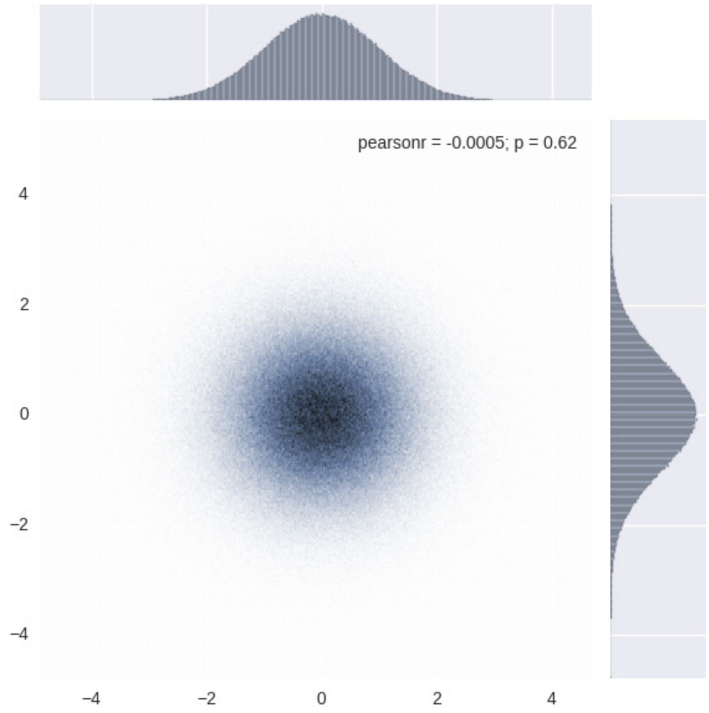
Sample covariance: $\bar{\sigma}_{i,j} = \dfrac{1}{N-1} \sum_{k=1}^{N} \left(x_i^{(k)} - \mu_i\right)\left(x_j^{(k)} - \mu_j\right)$

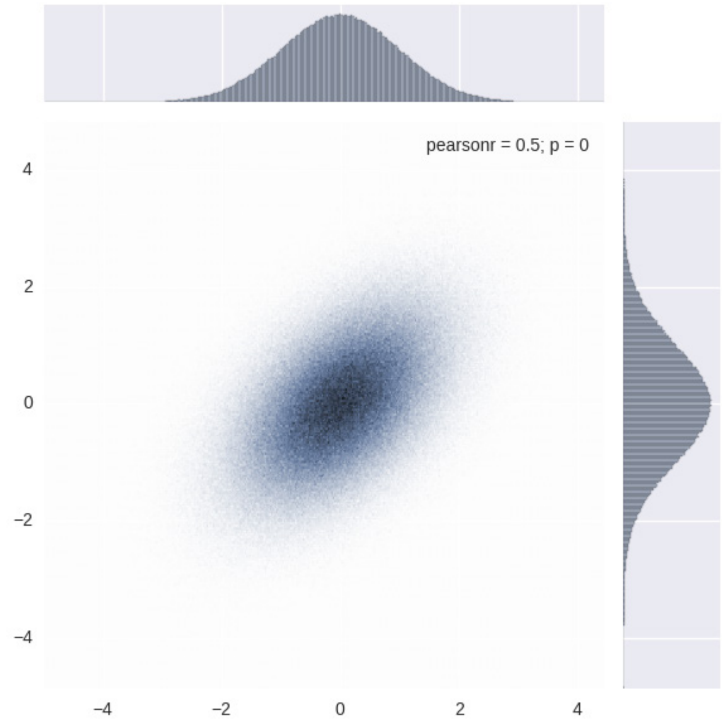
Covariance – 2D case



Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Covariance – 2D case





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Central Limit Theorem

"The sum of a number of independent and identically distributed random variables with finite variances will tend to a normal distribution as the number of variables grows."

$$\mu = \mathbb{E}\left[X_i\right]$$
$$\sigma^2 = \operatorname{var}\left[X_i\right]$$

$$M_n = \frac{1}{n}\sum_{i=1}^{n} X_i \xrightarrow{n\to\infty} \mathcal{N}\left(\mu, \sigma/\sqrt{n}\right)$$

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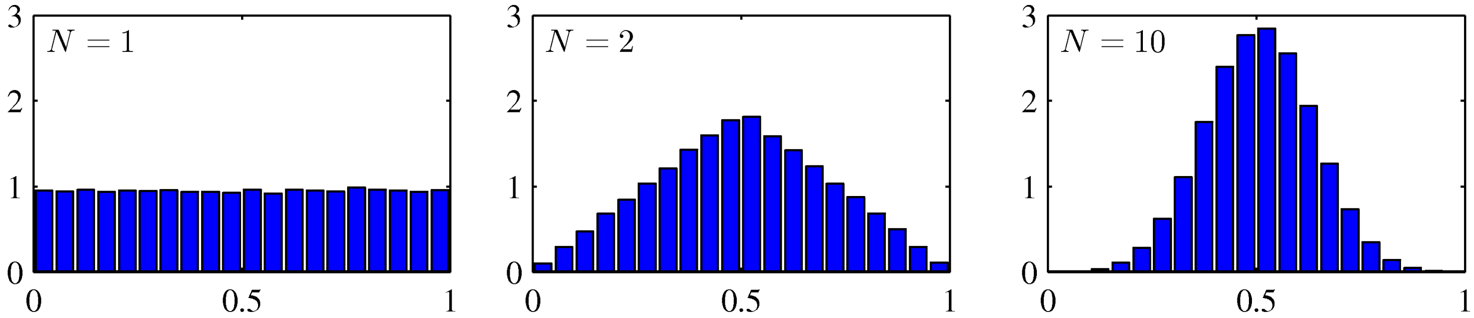

Bishop, sec. 2.3